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Flux gain for a next-generation neutron reflectometer resulting from improved supermirror performance

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Abstract. Next-generation spallation neutron source facilities will offer instruments with unprecedented capabilities through simultaneous enhancement of source power and usage of advanced optical components. The Spallation Neutron Source (SNS), already under construction at Oak Ridge National Laboratory and scheduled to be completed by 2006, will provide greater than an order of magnitude more effective source flux than current state-of-the-art facilities, including the most advanced research reactors. An additional order of magnitude gain is expected through the use of new optical devices and instrumentation concepts. Many instrument designs require supermirror neutron guides with very high critical angles for total reflection. In this contribution, we will discuss how the performance of a modern neutron-scattering instrument depends on the efficiency of these supermirrors. We summarize current limitations of supermirror coatings and outline ideas for enhancing their performance, particularly for improving the reflectivity at the critical wavevector transfer. A simulation program has been developed which allows different approaches for supermirror designs to be studied. Expected instrument performance gains are calculated for the example of the SNS reflectometer.

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The Spallation Neutron Source (SNS), currently under construction at Oak Ridge National Laboratory, will generate an effective neutron flux about one order of magnitude higher than the best existing neutron sources. Combined with further approaches to gain intensity by optimization of neutron optical components, development of new optical devices, and implementation of advanced instrument designs, an additional increase in flux by up to one order of magnitude should result for particular SNS scattering instruments [1]. The total intensity gain for SNS instruments, therefore, can be as high as two orders of magnitude, which will greatly enhance the quality of neutron scattering studies.

Supermirrors play an important role in most instrument designs at the SNS. We have theoretically analyzed the intensity gain that may be achievable for the SNS Magnetism Reflectometer by increasing the performance of its supermirror guide coatings. Our study is motivated by the fact that supermirror performance does not approach theoretical limits, particularly for mirrors of high critical angle.

1 Neutron guides and supermirrors

Neutrons can be very effectively transported by reflections on inner wall coatings of guide systems. A guide coating made of pure Ni is usually defined as an "$m = 1$" mirror. Supermirror coatings, consisting of depth-graded multilayers, allow to further increase the critical q value [2]. These structures are composed of thin films of materials showing large contrast in scattering length density, for example Ni and Ti. The performance of a supermirror (SM) is described by the increase of its q_c-value compared to natural Ni as $q_c^{SM} = m \times q_c^{Ni}$.

Supermirrors exceeding $m = 3.6$ became commercially available only recently after years of R & D at Paul Scherrer Institute (PSI)/Switzerland. A general drawback of high-m mirrors is that the reflectivity function of these coatings is far from being perfect (to a lesser extent this is also true for lower-m supermirrors, e.g. $m = 2$ and $m = 3$). In large-scale production of $m = 3.6$ supermirrors, for example, typical reflectivities of $R = 0.6 - 0.7$ are reached at q_c. The circles in Fig. 1 represent measured neutron reflectivity data from an $m = 3.6$ Ni/Ti supermirror [3].

Theoretically, assuming well-ordered layering, the reflectivity function should be considerably higher, on the order of 90% at q_c (cf. straight line). The calculation accounts for absorption due to the enormous total thickness of approximately 50 000 Å, incoherent scattering, and rms interfacial roughnesses of 10% of the adjacent layer thicknesses. Obviously, large performance losses are caused by imperfections at the Ni/Ti interfaces and by the surface roughness of the substrate.

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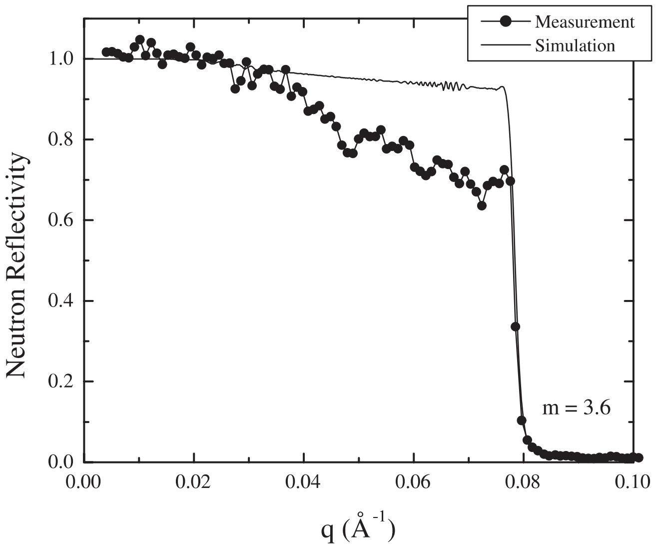

Fig. 1. Measured neutron reflectivity of an $m = 3.6$ supermirror compared with a calculation assuming 10% rms interfacial roughness (see text)

So far, interface diffusion and roughness effects are thought to be the main reasons for the low measured reflectivities; however, there might be other contributing factors that are not yet well investigated, for example small-angle scattering on the grain structure.

Major distortions to the reflectivity may also result from limited coherence due to deviations from the design layer thicknesses, as was pointed out by Mezei [4]. Positioning the interfaces near the nominal values in order to maintain coherent interference is quite a challenge, particularly for supermirrors with very high m-values and correspondingly small individual layer thicknesses. For example, in the case of an $m = 3.6$ supermirror, about 26 coherently reflecting bilayers are required for optimum reflectivity at q_c (where the individual layer thicknesses are about 40 Å). In order to satisfy the $\pm 45°$ phase difference criteria (cf. [4]), offsets of actual positions of interfaces must be less than 10 Å.

There have been some suggestions recently to avoid amplification of interface roughness that occurs naturally when several hundred bilayers are being deposited. One idea is to smooth the layers after a certain fraction of the total deposition process. For example, Soyama et al. have applied ion polishing in combination with ion beam sputtering [5]. They achieved a decrease in the rms roughness of Ni films by ion-polishing from 6.5 Å to 3.5 Å.

2 Performance gains for the SNS neutron reflectometer

This section demonstrates expected gains in the instrument performance of the proposed SNS Magnetism Reflectometer (see [6] for a more detailed description), which may be achievable by improving high-m supermirror coatings. The basic layout of the instrument is illustrated in Fig. 2. Neutrons from the cold liquid hydrogen moderator are guided to the sample position at an 18 m distance via a combination of a channel beam bender and a tapered neutron guide. The bender (length: 5 m) is used to minimize high-energy neutron background at the sample position. It deflects the useful part of the wavelength distribution ($\lambda > 1.5$ Å) by about 2° horizontally and feeds it into a 9 m long focusing section, which compresses the beam size to match a typical sample size of 25 mm × 25 mm. High-energy neutrons cannot follow this curvature and are scattered and absorbed by appropriate shielding. Neutrons scattered by the sample will be counted by a two-dimensional multidetector at a 19 m distance from the moderator. The wavelength is determined by time-of-flight. The instrument is designed for 60 Hz operation, the normal source frequency of SNS. Bandwidth choppers restrict the total bandwidth of neutrons that are incident onto the sample to $\Delta\lambda = 3.5$ Å. If, for example, the most intense wavelength band from 2.6 Å to 6.1 Å is used for data collection at the SNS instrument, a neutron flux of approximately 3.7×10^9 neutrons/cm^2/s (at guide exit) can actually be used for concurrent data collection.

The neutron guide system of the instrument has been optimized by Monte Carlo simulations using the program IDEAS [7]. The above stated flux number implies that $m =$

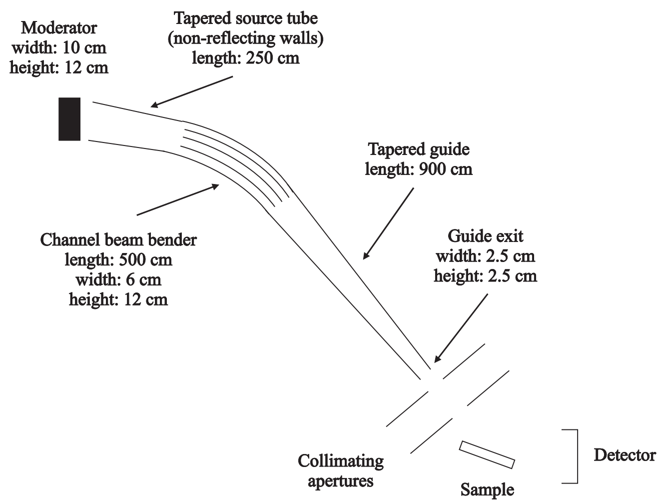

Fig. 2. Schematic layout of the Magnetism Reflectometer to be built at SNS (plan view)

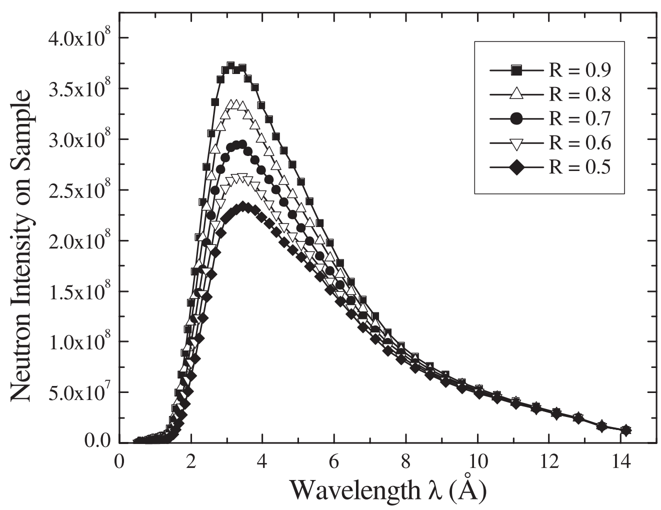

Fig. 3. Effect of different reflectivity (R) values (at q_c) for $m = 3.5$ supermirrors on simulated Magnetism Reflectometer neutron guide performance

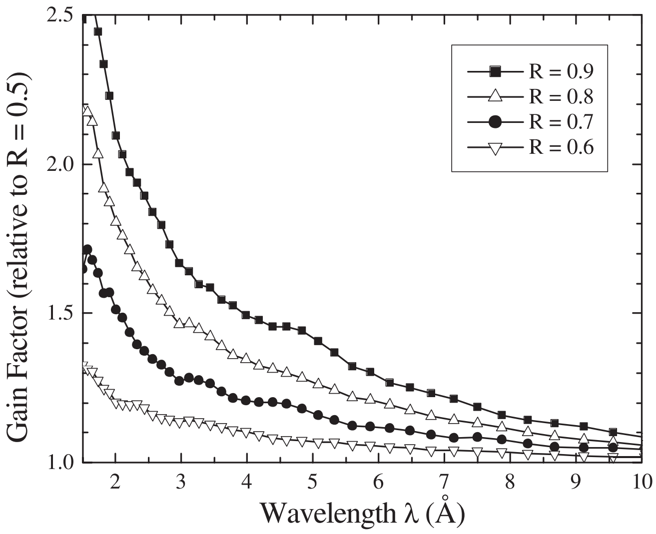

Fig. 4. Neutron intensity gain of various supermirror guide coatings (with different R-values at q_c) relative to an $R = 0.5$ coating

3.5 supermirrors with 65% reflectivity at the critical edge will be utilized for all guide surfaces. This specification is challenging but does not seem to be beyond the capabilities of current guide vendors.

Figure 3 shows the effect of varying the reflectivity value (at q_c) for the above instrument configuration in the wavelength range up to 14 Å. The reflectivity below q_c^{Ni} was assumed to be $R = 0.98$, followed by a linear decrease between q_c^{Ni} and q_c^{SM}. In order to reflect a realistic situation in which large guide gains can be expected, we calculate flux on sample for a low-resolution, high-q experiment. In this case a highly divergent beam can be utilized. In particular, we assume: 25 mm × 25 mm sample size, 20° incident angle, and 10% angular resolution. The latter is achieved by using a pair of slits with 0.5 m distance from each other, which is located between the exit of the tapered guide and the sample position. The intensities displayed in Fig. 3 have been integrated over 5% wide neutron wavelength bins. Note that the sharp wavelength cut-off at about 2 Å results from using the beam bender.

Figure 4 shows relative enhancements in flux-on-sample achievable if supermirrors with higher reflectivity at q_c can be produced in large quantities. The intensity gain functions have been calculated by normalizing the flux values of Fig. 3 relative to the $R = 0.5$ data. As can be seen from Fig. 4, the intensity, particularly at short wavelengths, would be significantly increased.

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References

1. R.K. Crawford: Proc. of ICANS-XV **61**, (2000)
2. P. Boeni, D. Clemens, M. Senthil Kumar, S. Tixier: Physica B **241–243**, 1060 (1998)
3. M. Senthil Kumar, P. Boeni, D. Clemens: J. Appl. Phys. **84**, 6940 (1998)
4. F. Mezei: In *Physics, Fabrication, and Applications of Multilayered Structures* (Plenum Press, New York 1987) p. 311
5. K. Soyama, W. Ishiyama, K. Murakami: JAERI-Review 2000-005, **57** (2000)
6. W.-T. Lee, F. Klose: In Neutron Optics, ed. by J.L. Wood, J.S. Anderson, Proc. SPIE Vol. 4509 (2001) pp. 145–156
7. W.-T. Lee, J.L. Robertson, D.-Q. Wang, M.L. Crow, F. Klose: IDEAS – A Monte Carlo simulation package for neutron scattering instrumentation. J. Appl. Phys. A **74**, this issue (2002)